

# Stretched exponentials in the dynamics and at the ground state of the plaquette Ising model

Adam Lipowski<sup>1</sup>

<sup>1</sup>*Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland*

Simulations show that the autocorrelation function  $C(t)$  in the  $d = 3$  Ising model with a plaquette interaction has a stretched-exponential decay in a supercooled liquid phase. Such a decay characterizes also some ground-state probability distributions obtained from the numerically exact counting of up to  $10^{450}$  configurations. A related model with a strongly degenerate ground state but lacking glassy features does not exhibit such a decay. Tensionless modification of the droplet model might explain stretched-exponential decay of  $C(t)$  even in three-dimensional systems.

Assuming that liquids constitute a homogeneous and continuum medium, one can explain many of its properties such as viscosity, diffusion or chemical reaction rates. However, cooling below melting point causes drastic changes in the dynamics and a homogeneous approach is no longer legitimate [1]. One of the landmarks of this supercooled regime is a slower than exponential decay of autocorrelation functions. Although this decay is often fitted with the so-called stretched exponentials  $\exp[-(t/\tau)^\beta]$ , it is sometimes questioned as being merely a phenomenological fit to experimental data without any clear microscopic mechanism [2].

It is becoming commonly accepted that supercooled liquids are dominated by dynamically generated heterogeneities. They have different sizes and lifetimes and their dynamics is thus very complex. It would be desirable to relate this dynamics with some kind of an Ising model the dynamics of which is relatively understood. Particularly interesting in this context might be the droplet model, which predicts in some cases the stretched-exponential decay of autocorrelation functions [3]. According to the droplet model, however, such a decay should hold only for low-dimensional Ising systems, and in the most interesting three-dimensional case, an exponential decay is expected.

A promising statistical mechanics approach to glassy systems refers to lattice models. Various models of glasses, including kinetically constrained or spin-facilitated ones have already been examined [4]. Although they exhibit an interesting slow dynamics, their thermodynamics is very often trivial. A more comprehensive description of glasses might be thus sought among Ising models.

In the present Letter, we examine the Ising model with plaquette interaction, that is defined using the following Hamiltonian

$$H = - \sum_{(i,j,k,l)} S_i S_j S_k S_l, \quad S_i = \pm 1, \quad i = 1, 2, \dots, L^d \quad (1)$$

where summation is over elementary plaquettes of the  $d$ -dimensional Cartesian lattice of the linear size  $L$  with periodic boundary conditions. For  $d = 3$ , model (1) shares a number of properties with glassy systems. In partic-

ular, it exhibits a strong metastability [5, 6] and a very slow (perhaps logarithmically slow) coarsening dynamics [7]. Moreover, aging [6] and cooling-rate effects [8] are consistent with expectations for ordinary glasses. Let us also notice that even the  $d = 2$  version of the model, despite trivial thermodynamics, exhibits an interesting glassy behaviour [9, 10].

To examine the dynamics of model (1) in the supercooled liquid phase, we calculated the spin-spin autocorrelation function that is defined as

$$C(t) = \frac{1}{L^3} \sum_i \langle S_i(0) S_i(t) \rangle \quad (2)$$

Using a standard Metropolis dynamics, we simulated the model for the  $d = 3$  case at several temperatures and measured  $C(t)$ . The results of these simulations are shown in Fig.1. Fitting our data to the function  $a \exp[-(t/\tau)^\beta]$ , we obtained the exponent  $\beta$ , and its temperature dependence is shown in the inset. Let us notice that earlier studies of model (1) locate the glassy transition close to  $T = T_g \approx 3.4$  and the first-order melting transition (located on the comparison of free energies and simulations with nonhomogeneous initial conditions) around  $T = T_m \approx 3.6$  [5, 6, 11]. One can notice that for  $T < T_m$  an appreciable departure from the exponential ( $\beta = 1$ ) decay is seen. It is not clear to us whether  $\beta$  becomes smaller than 1 precisely at  $T_m$  or at a somewhat larger value, as our data might suggest. Studies of long-time evolution of glassy systems using molecular dynamics simulations of realistic systems are computationally very demanding, but in a model with a controlled frustration, Shintani reported a similar temperature dependence of  $\beta$  [12]. A stretched-exponential behaviour of the energy autocorrelation function with  $\beta$  decreasing upon approaching  $T_g$  has already been reported for model (1) [6]. However, energy is a global variable and it is not clear whether such a quantity correctly probes the heterogeneous dynamics of supercooled liquids. There are also some reports of a stretched exponential behaviour in other Ising-like lattice models with glassy features [13] but it might be a consequence of a reduced ( $d = 2$ ) dimensionality, which according to the droplet model [3] might imply such a decay of  $C(t)$ .

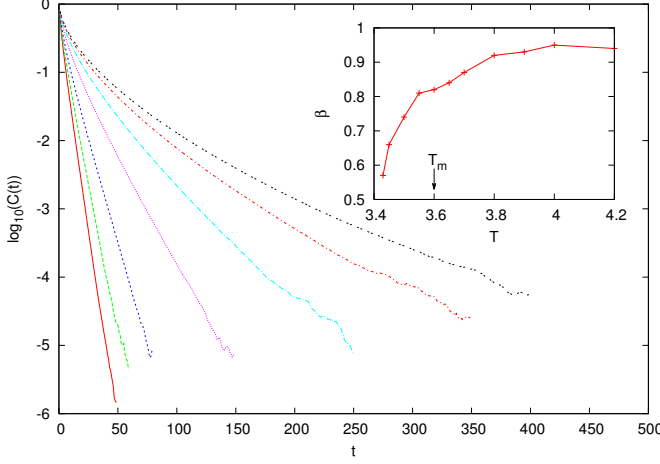


FIG. 1. The time dependence of the spin-spin autocorrelation function  $C(t)$  for (from above)  $T = 3.43, 3.45, 3.5, 3.6, 3.8, 4.0$ , and  $4.2$ . At each temperature, simulations start from a random initial configuration, which is relaxed for a certain time ( $\sim 10^3$ ), and then measurements are made during  $t \sim 10^7$  ( $L = 50$ ). A unit of time corresponds to a single on average update per spin. The inset shows the exponent  $\beta$  obtained from the fit to the stretched exponential ( $a \exp -(t/\tau)^\beta$ ). The arrow indicates location of the first-order melting transition in the model.

As we show below, stretched exponentials appear in model (1) also in a much different context. Namely, they characterize some ground-state probability distributions. A calculation of these distributions is possible because a strongly degenerate ground state has in fact a relatively simple structure. For example, for  $d = 2$  all its configurations can be obtained from a reference configuration (e.g., all spins  $+$ ) by flipping vertical and horizontal rows of spins (Fig.2), which leads to its  $2^{2L-1}$  degeneracy [9].

To illustrate the calculations, let us examine the susceptibility-like variable  $\chi_2 = \frac{1}{L^2} \sum_{i,j} S_i S_j = \frac{1}{L^2} (\sum_i S_i)^2$ . One can notice that to calculate  $\chi_2$  precise distribution of these flipped rows is not needed, and it is sufficient to know only their numbers  $k_1$  and  $k_2$ . Indeed, flipping  $k_1$  horizontal rows, we reduce the number of  $+$  spins to  $N_+ = L^2 - k_1 L$ . The subsequent flip of  $k_2$  vertical rows leads to  $N_+ = L^2 - (k_1 + k_2)L + 2k_1 k_2$ . Using  $\sum_i S_i = 2N_+ - L^2$ , we obtain that for  $(k_1, k_2)$  configurations  $\chi_2 = \frac{1}{L^2} [L^2 - 2(k_1 + k_2)L + 4k_1 k_2]^2$ . Of course, calculating the probability distribution of  $\chi_2$ , one should take into account the multiplicity factor equal to  $\binom{L-1}{k_1} \binom{L-1}{k_2}$ .

The above considerations can be easily generalized to the  $d = 3$  version. In this case, ground-state configurations can be obtained from the reference configuration by flipping entire two-dimensional planes. To characterize a given ground-state configuration, we now need three

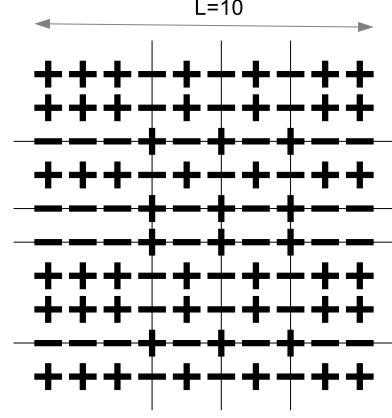


FIG. 2. An example of a ground-state configuration in the  $d = 2$  case obtained from the ferromagnetic state (all  $+$ ) by flipping  $k_1 = 4$  horizontal and  $k_2 = 3$  vertical rows of spins.

numbers  $(k_1, k_2, k_3)$ , for which we obtain

$$\chi_3 = \frac{1}{L^3} [L^3 - 2(k_1 + k_2 + k_3)L^2 + 4(k_1 k_2 + k_1 k_3 + k_2 k_3)L - 8k_1 k_2 k_3]^2. \quad (3)$$

The corresponding multiplicity factor equals  $\binom{L-1}{k_1} \binom{L-1}{k_2} \binom{L-1}{k_3}$ .

For a further analysis of the probability distribution, we resort to numerical calculations. For  $d = 3$  and a given system size  $L$ , we generate all  $(L-1)^3$  triples  $(k_1, k_2, k_3)$ , and using Eq.(3), we calculate  $\chi_3$  and the corresponding multiplicity factor. Collecting the data in some bins, we obtain the required probability distribution  $P(\chi_3)$ . Let us notice that computational complexity of generation of such triples is rather modest ( $\sim L^3$ ), which allows us to examine large systems ( $L \sim 500$ ) within few seconds of CPU time.

The results presented in Fig.3 show that  $P(\chi_3)$  has a maximum at  $\chi = 0$ . Let us notice, however, that the average over all ground-state configurations  $\langle \chi_3 \rangle = 1$ . This is a consequence of the flipping symmetry of the Hamiltonian (1), which implies that for any  $i \neq j$  the corresponding correlation function  $\langle S_i S_j \rangle$  vanishes [5]. The only nonvanishing contribution to susceptibility comes from the case  $i = j$  and that implies  $\langle \chi_3 \rangle = 1$ .

The above symmetry arguments are valid also at finite (and sufficiently high) temperature and recent Johnston's Monte Carlo simulations report indeed  $\langle \chi_3 \rangle \approx 1$  [14]. These simulations also show that at low temperature the susceptibility drops almost to zero. Our results (Fig.3) shed some light on such a finding: Monte Carlo simulations at low temperature select randomly one of the ground states (toward which the system slowly evolves) and since  $\chi_3 = 0$  is the most probable value in  $P(\chi_3)$ , this is the value that is typically measured in Monte Carlo simulations. Let us notice that due to the strong degeneracy of the ground state, it is difficult to find the order parameter that would distinguish low and high temperature

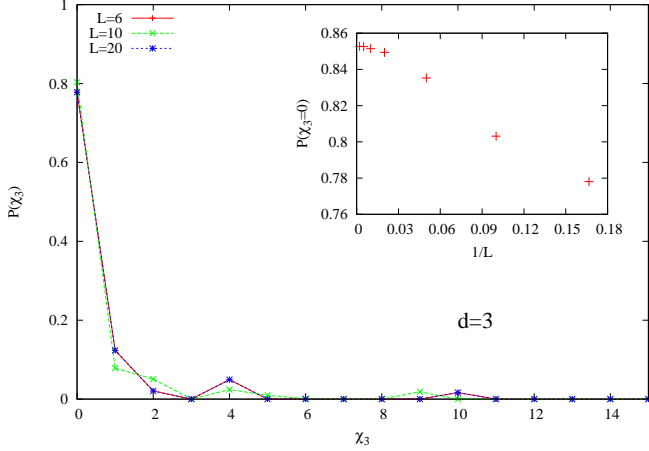


FIG. 3. The probability distribution for the susceptibility  $\chi_3$ . The fact that  $\chi_3 = 0$  is the most typical value of these distributions agrees with the recent Monte Carlo simulations for lattices of similar size showing that at low temperature the susceptibility drops to zero [14]. The inset shows  $P(\chi_3 = 0)$  as a function of  $1/L$  for  $L = 6, 10, \dots, 500$ .

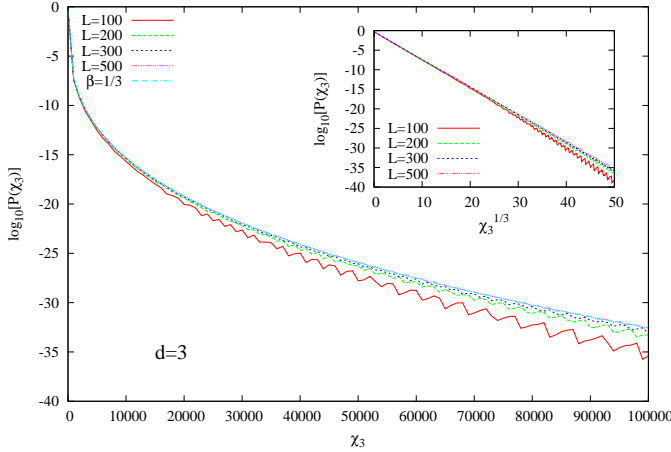


FIG. 4. Logarithm of the probability distribution  $P(\chi_3)$  for the three-dimensional version. For  $L = 500$ , the data nearly overlap with the least-square fit with  $\beta = 1/3$ . The inset confirms the stretched exponential decay with  $\beta = 1/3$  for nearly 120 decades.

phases of the model (1). Johnston's result suggests that the susceptibility might serve as such, but  $P(\chi = 0)$  for increasing  $L$  does not converge to unity (inset in Fig.3) and there is a finite (albeit small) probability that simulations will select the ground state with  $\chi > 0$ .

Further analysis of  $P(\chi_3)$  (Fig.4) shows a slower than exponential decay for large  $\chi_3$ . Plotting against  $\chi_3^{1/3}$  shows an excellent linearity of the data for nearly 120 decades and indicates that asymptotically  $P(\chi_3)$  decays as stretched exponential  $\exp(-a\chi_3^{1/3})$ . Let us also notice that for  $L = 500$  the obtained probability distribution is based on the (numerically) exact counting of  $2^{3 \cdot 500 - 2} \sim 10^{450}$  ground-state configurations.

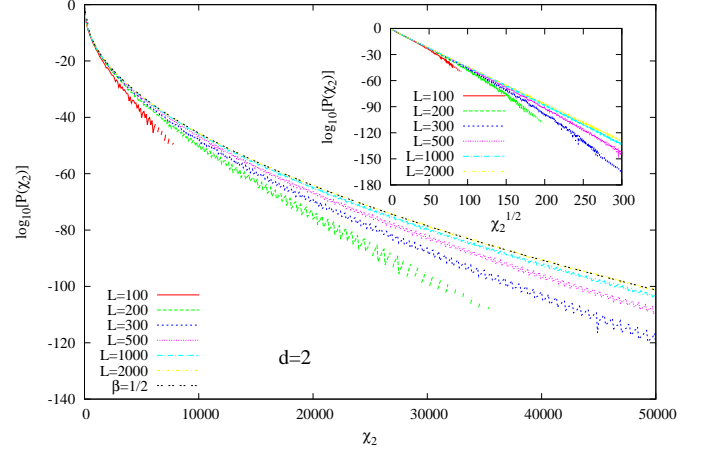


FIG. 5. Logarithm of the probability distribution  $P(\chi_2)$  for the two-dimensional version. For  $L = 2000$ , the data nearly overlap with the least-square fit with  $\beta = 1/2$ . The inset confirms the stretched exponential decay with  $\beta = 1/2$  for nearly 120 decades.

Although the  $d = 2$  version of the model (1) has a trivial thermodynamic behaviour, it exhibits an interesting glassy-like dynamic behaviour [9]. Calculating the distribution  $P(\chi_2)$ , we also find the stretched exponential decay but with the exponent  $\beta = 1/2$  (Fig.5).

It is not clear to us whether stretched exponential (static) distributions that we found at the ground state of model (1) are related at all with its finite-temperature dynamic behaviour. However, a curious example comes from a more general version of model (1) known as the gonihedric model. This model, introduced in the context of the discretized string theory [15], is described by the following Hamiltonian

$$H = -2\kappa \sum_{i,j} S_i S_j + \frac{\kappa}{2} \sum'_{i,j} S_i S_j - \frac{1-\kappa}{2} \sum_{(i,j,k,l)} S_i S_j S_k S_l \quad (4)$$

where the first and the second summations are over the nearest and the next-nearest neighbours, respectively. For  $\kappa = 0$ , the model reduces to the plaquette model (1). A quite different thermodynamic and dynamic behaviour is reported for  $\kappa \neq 0$  [7, 16]. In such a case, there is no metastability upon temperature changes and the dynamics does not exhibit glassy features. Also the flipping symmetry of the model (4) is lower than in the case of  $\kappa = 0$ . In particular, flipped planes or rows of spins cannot cross [16]. This simplifies the calculations we made for the plaquette model since now only one of the numbers  $k_1, k_2$  or  $k_3$  might be nonzero. In the  $d = 3$  version of the gonihedric model for a configuration with  $k$  planes flipped, we thus obtain

$$\chi_{3\kappa} = \frac{1}{L^3} [L^3 - 2kL^2]^2 = L[L - 2k]^2. \quad (5)$$

and the multiplicity factor being equal to  $3 \binom{L}{k}$  (with

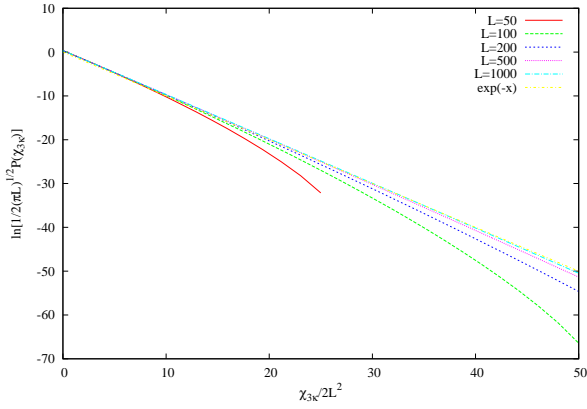


FIG. 6. Rescaled logarithm of the probability distribution  $P(\chi_{3\kappa})$  for the three-dimensional version of the gonihedric model (4) for  $\kappa \neq 0$ . For  $L = 1000$ , the data nearly overlap with the straight line corresponding to  $\exp(-x)$  confirming thus the asymptotic estimation (7).

prefactor 3 corresponding to the number of directions of flipped planes). Using the above equation, one obtains

$$P(\chi_{3\kappa}) = \frac{6}{3 \cdot 2^L} \binom{L}{\frac{1}{2}(L - \sqrt{\chi_{3\kappa}/L})} \quad (6)$$

where  $3 \cdot 2^L$  is the degeneracy of the ground state. Using the identity  $\binom{L}{k} = \frac{(L/2)!(L/2)!}{(L-k)!k!}$  and the asymptotic form  $\binom{L}{L/2} \approx \frac{2^L}{\sqrt{\pi L}}$ , after some calculations one obtains that for  $1 \ll \sqrt{\chi_{3\kappa}/L} \ll L$

$$P(\chi_{3\kappa}) \approx \frac{2 \exp(-\frac{\chi_{3\kappa}}{2L^2})}{\sqrt{\pi L}} \quad (7)$$

Our numerical data are in a very good agreement with the above estimation (Fig.6). Let us notice that  $P(\chi_{3\kappa})$  has an exponential decay that in the thermodynamic limit  $L \rightarrow \infty$  flattens and  $P(\chi_{3\kappa}) \rightarrow 0$ . Thus the ground-state distribution in the gonihedric model for  $\kappa \neq 0$  has a much different form than in the  $\kappa = 0$  case. Perhaps it is only a coincidence that in the latter case, where the model exhibits glassy behaviour, the distribution  $P(\chi_3)$  has a stretched-exponential behaviour. But one cannot exclude a more profound relation between zero-temperature statics and finite-temperature dynamics of model (1).

In the final part of our Letter, we would like to return to the problem of the decay of  $C(t)$  in the supercooled regime. It would be desirable to explain such a dynamics in terms of some kind of the droplet model [3]. The droplet model most likely provides a qualitatively correct description of the Ising dynamics [17] but it predicts the exponential decay of  $C(t)$  for  $d = 3$  systems. It seems to us, however, that trying to use the droplet model to explain the dynamics of model (1), we might have to modify some of its assumptions. Indeed, the excess energy  $e_l$  of a

droplet of linear size  $l$ , which for an ordinary Ising model is proportional to its surface ( $e_l \sim l^{d-1}$ ), in model (1) might scale as  $e_l \sim l^{d-2}$  [5, 16]. Actually, droplets with energy proportional to  $l^{d-1}$  are also possible in model (1) but in our opinion the long-term dynamics might be under the influence of mainly the (low-energy) tensionless droplets. Assuming  $e_l \sim l^{d-1}$  and repeating Lifshitz reasoning, one obtains that the deterministic motion of a droplet satisfies  $dl/dt \sim l^{-2}$  and the resulting lifetime of a domain of the initial size  $l$  thus scales as  $l^3$ . Consequently, the form of the Boltzmann factor leads to the estimation  $C(t) \sim \exp[-(t/\tau)^{(d-2)/3}]$ . Thus, tensionless domains in model (1) might imply stretched exponential behaviour in three-dimensional systems.

The dynamics of model (1) in the supercooled liquid phase is very complex and most likely the entire spectrum of droplets is present. Droplets with energies scaling as  $l^{d-2}$  and  $l^{d-1}$  are only limiting cases and perhaps a more adequate description could be obtained assuming  $e_l \sim l^\phi$ , where  $d-2 < \phi < d-1$ . In such a case, we are lead to  $C(t) \sim \exp[-(t/\tau)^{\phi/(d+1-\phi)}]$ . In our opinion, it would be desirable to calculate surface tension of droplets in model (1) possibly confirming their tensionless nature.

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